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SPARSE AEROSOL MODELS BEYOND THE QUADRATURE METHOD OF MOMENTS

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Extended Abstract

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Sparse Aerosol Models Beyond the Quadrature Method of Moments

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Abstract. This study examines a class of sparse aerosol models derived from linear programming (LP). The widely used quadrature method of moments (QMOM) is shown to fall into this class. Here it is shown how other sparse aerosol models can be constructed, which are not based on moments of the particle size distribution. The new methods enable one to bound atmospheric aerosol physical and optical properties using arbitrary combinations of model parameters and measurements. Rigorous upper and lower bounds, e.g. on the number of aerosol particles that can activate to form cloud droplets, can be obtained this way from measurement constraints that may include total particle number concentration and size distribution moments. The new LP-based methods allow a much wider range of aerosol properties, such as light backscatter or extinction coefficient, which are not easily connected to particle size moments, to also be assimilated into a list of constraints. Finally, it is shown that many of these more general aerosol properties can be tracked directly in an aerosol dynamics simulation, using sparse aerosol models, in much the same way that moments are tracked directly in the QMOM.

Keywords: Atmospheric aerosols, Sparse aerosol models, Aerosol physical and optical properties, Aerosol dynamics, Quadrature Method of Moments
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INTRODUCTION

Models by their very nature tend to be sparse in the sense that they are designed with very few optimally selected parameters to provide simple yet faithful representations of a complex observational dataset or detailed computer simulation. In addition to accuracy, a well-designed sparse model naturally has advantages for economy of representation and great computational speed.

Sparse aerosol representations include sectional, modal, and moment models whereby the aerosol is classified into a basis consisting of a typically small number of size sections, modes, or moments. For our purposes, the term "sparse" will refer to the replacement of an essentially continuous particle size/composition population by a (typically small) set of delta functions or abscissas and weights.

Moment methods have rich mathematical connections to orthogonal polynomials, continued fractions, and quadrature. In the quadrature method of moments (QMOM) [1] a sequence of e.g. radial moments is defined in terms of the distribution function $f(r)$ by:

$$\mu_k = \int_0^\infty r^k f(r)\,dr \approx \sum_{i=1}^{N} (r_i)^k w_i \quad . \tag{1}$$

These moments may be inverted using matrix methods [2] to obtain quadrature abscissas, r_i, and weights, w_i, cf. the approximate equality of Eq. 1. For $2N$ moments and N abscissa and weight pairs the result is exact. Knowledge of the distribution function is not required for quadrature, only its lower-order moments [1]. Aerosol physical and optical properties can be estimated simply in terms of the quadrature set. For a generic property M_k, linear in the particle distribution function, we have in analogy with Eq. 1:

$$M_k = \int_0^\infty \sigma_k(r) f(r)\,dr \approx \sum_{i=1}^{N} \sigma_k(r_i) w_i \tag{2}$$

where $\sigma_k(r)$ is a known kernel function, such as a light extinction kernel, and the abscissas and weights have the same values as in Eq. 1. Clearly, for $\sigma_k(r) = r^k$ Eq. 2 reduces to Eq. 1. The basis of the QMOM is the idea that not only can aerosol properties be estimated this way directly from moments, but the aerosol dynamical equations themselves can be cast in terms of quadrature, a feature that allows for closure of the moment evolution equations without need to know $f(r)$: Only the sparse quadrature representations of $f(r)$ need be carried through in models – a fact that makes the QMOM a highly efficient, as well as highly accurate, computational method [1].

In a subsequent paper on time-dependent correlation functions, Platz and Gordon showed how the moment inversion problem can be handled by linear programming as well as by matrix methods [3]. This is an important observation because LP is *not* a moment method, but one that allows a more diverse range of kernels to be handled in the same manner that moments are handled in the QMOM. The purpose of the present study is to follow up on this idea with a preliminary exploration of its potential for expanding applications of sparse particle models in aerosol science.

RECOVERY OF THE QMOM USING LINEAR PROGRAMMING

The linear programming problems discussed here are of the general form:

Minimize cost function:	$\mathbf{c} \cdot \mathbf{w}^{\mathbf{T}}$	
Subject to equality constraints:	$\mathbf{a_k} \cdot \mathbf{w}^{\mathbf{T}} = \mathbf{M_k}$	(LP)
Together with	$w_i \geq 0$	

Here $\mathbf{w} = \{w_1, w_2, \cdots, w_n\}$ is a vector of variable amplitudes, such as the number of particles at grid location r_i, and n is the number of grid locations. Unlike the QMOM, the LP- sparse aerosol models require a grid, but that grid is adaptable (location placements are arbitrary) and the dimensionality of the grid is also arbitrary (i.e. each r_i can be a vector containing multiple aerosol size/composition coordinates). $\mathbf{c} = \{c_1, c_2, \cdots, c_n\}$ is the vector of cost function coefficients. Each of the equality constraints takes the form

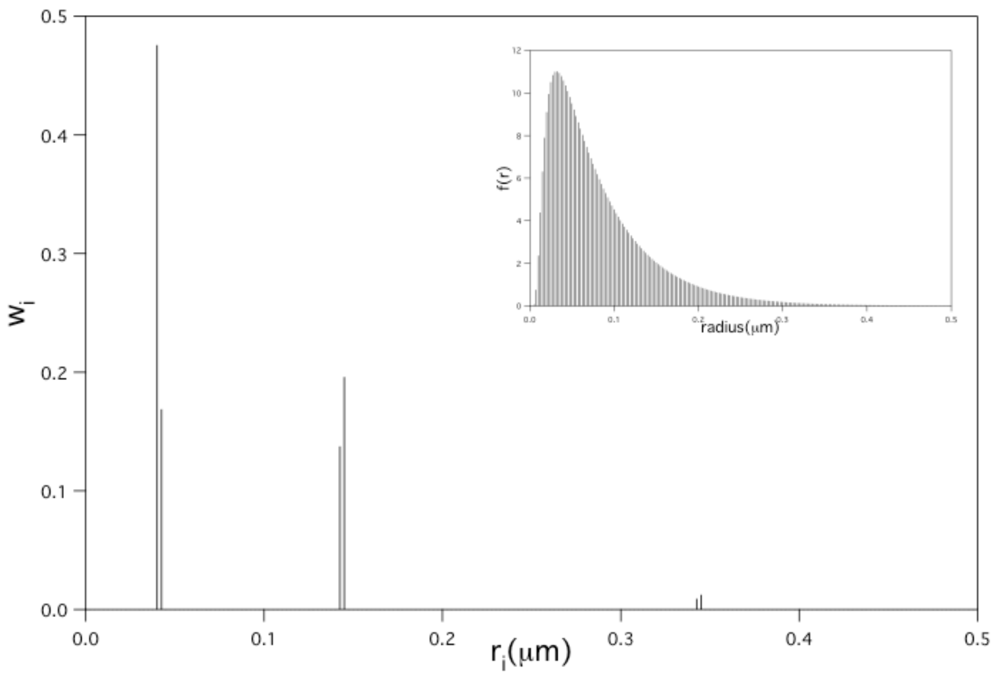

FIGURE 1. Quadrature abscissas and weights obtained by constraining the first 6 integral moments to those of the test aerosol distribution shown in the insert. The test distribution is from Hoppel et al. [4] and is their distribution #4. The three quadrature points are split among neighboring grid points due to limited resolution of the grid. Otherwise perfect agreement with QMOM matrix-based moment inversion is obtained.

$\mathbf{a_k} \cdot \mathbf{w^T} = \mathbf{M_k}$ for some specified moment or measurement k having the structure of the middle term in Eq. 2 where $\mathbf{a}_k = \{a_{k1}, a_{k2}, \cdots, a_{kn}\}$ derives from the kernel. Because of their similar structures, the cost function and any one of the equality constraints are interchangeable. Thus one can bound a moment, such as particle surface area or volume, using a set of extinction measurements, or one can predict bounds for an extinction measurement from specified values of moments and/or other measurements.

Figure 1 illustrates application of the method for an aerosol test distribution studied by Hoppel [4]. The QMOM quadrature points are recovered on bounding the Laplace transform of $f(r)$ [5]. Thus the cost function elements are $c_i = e^{-r_i s}$. The results are independent of transform variable s, which we set for convenience to the inverse mean particle size, $= \mu_0 / \mu_1$. For equality constraints we use the first six integral moments calculated from the Hoppel test distribution, $\{\mu_0, \mu_1, \cdots, \mu_5\}$, with $\mu_0 = 1$ for the normalized distribution. The grid consists of $n = 201$ points evenly spaced over the radial coordinate from 0 to 0.5 micron. Figure 1 shows the sparse solution resulting from solving LP. The insert shows the original distribution. Of all the possible feasible aerosol distributions (positive abscissas, positive weights, and satisfaction of the constraint set) the solution shown here minimizes the discrete Laplace transform. Minimizing, instead, $-\mathbf{c} \cdot \mathbf{w^T}$ maximizes the cost function; providing a second sparse solution (not shown), and an upper bound to the Laplace transform consistent with the constraint set.

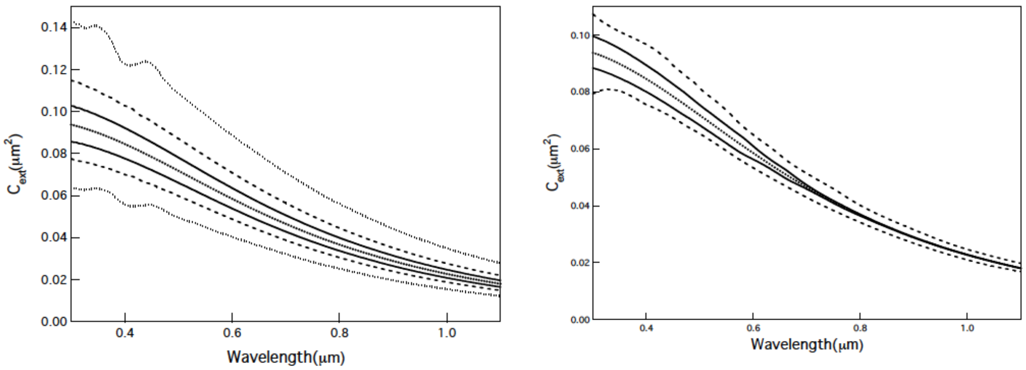

FIGURE 2. Nested pairs of upper and lower bounds to the extinction coefficient: Left panel derives from partitioning the Hoppel distribution into various numbers of equally-spaced size sections between 0 and 0.5 microns and using the known particle number concentrations in each section as LP constraints. Dotted, dashed, and solid bounds are from partitioning into 10, 20, and 40 sections, respectively. Right panel tests the effect of moment constraints. Dashed and solid bounds are derived using the first 6 and 20 integer-order radial moments, respectively. Center curves in each figure give the extinction coefficient for the Hoppel test distribution as a function of wavelength from Mie theory.

EXAMPLE: COMPARING OPTICAL EXTINCTION COEFFICIENT BOUNDS FOR SECTIONAL VS MOMENT CONSTRAINTS

The next examples test application of sparse aerosol models to data assimilation problems beyond capability of moment methods [6]. Nested bounds to the Mie scattering extinction coefficient are shown in Fig. 2. LP calculations were carried out at 161 evenly spaced wavelengths between 0.3 and 1.1 micron, using a value of 1.55 for the particle refractive index. For each wavelength upper and lower bounds were computed - a total of 322 separate LP calculations for each bound pair. Left panel bound pairs derive from particle occupation number constraints for sectional models of differing resolution (see caption). The extent to which the bounds are refined through a doubling and then quadrupling of the number of sections provides a quantitative measure of information achievable through sub-grid resolution. Number constraints are replaced by moment constraints in the right panel as described in the caption.

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